

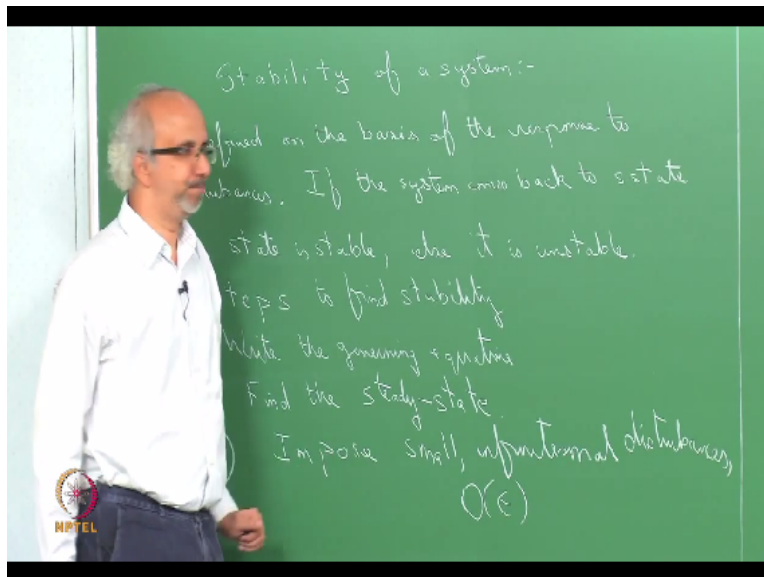
Multiphase Flows: Analytical Solutions and Stability Analysis
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Lecture – 21
Stability of distributed systems (PDEs): reaction diffusion example

So welcome to this lecture on multiphase flows. We saw some introductory concepts about stability analysis in the last class. If Jason spoke about 2-dimensional system and he took an example and he just worked out how you go about calculating the stability of a system and especially if there is a parameter working in the system, then that parameter would be something which you can control as an experimentalist.

And what you want to do is, you want to find out how the stability of a system changes as you vary that parameter. So that parameter could be flow rate, it could be temperature, it could be concentration, okay. So like it was mentioned in the last class, what we really have to do as far as finding stability of a system, I mean, it is decided by the response to perturbations, response to disturbances, right.

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This is defined on the basis of the response to disturbances. The idea is if we give a disturbance and if a system deviates from the steady-state, you say it is unstable. If it comes back to a steady-state, you say it is stable, okay. So if the system comes back to the steady-state, the state is stable,

else it is unstable. So I just want to emphasize again when I am talking about stability, I am talking about stability of a state, okay.

Now this is what you understand in English what we want to do is we want to develop a mathematical framework and what we got is some idea about the mathematical framework in the context of system of 2 variables which are dependent only on time but not on space. So just to keep the mathematics simple, so the example that was illustrated in the last class was that of 2 ordinary differential equations.

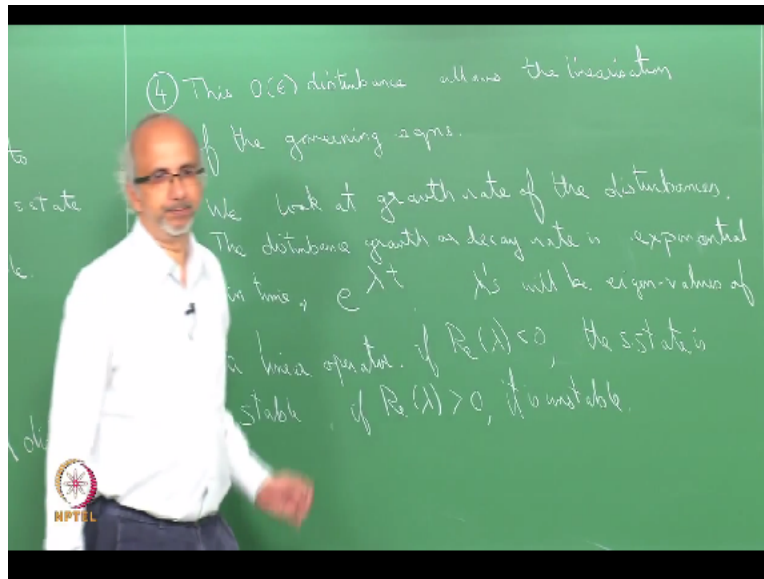
So you need the time dependency because whenever you are talking about stability, you are talking about response with respect to time. So you always are talking about an unstable or an unsteady-state system, okay and therefore, you need the time dependency to keep the maths simple, we made it well stirred and then you will neglect every spatial variations. So the basic idea, so whenever you want to find out the stability of a system, what are the steps you need.

The steps to find stability is first write the governing equations. This could be continuity equation, momentum conservation of mass, whatever it is, we are not going to describe the system, okay. Then once you have the governing equations, what is the next thing you have to do. The next thing I have to do is find the steady-state, okay and this would be dependent upon the problem you have considered in the first step.

Second thing is find the steady-state, okay because it is the stability of the steady-state which we are interested in. So we will find the steady-state whose stability you are talking about and then what do we do? We spoke about disturbances being given. So what we want to do is we want to give disturbances to the steady-state, okay and what we do is we impose small, when I say small, I mean infinitesimal, disturbances and here is where the order of epsilon comes in.

So these are basically of order epsilon, very small disturbances and that is the connection which I want you to make with the perturbation series, thing that you have seen earlier when you are trying to actually do things that are order epsilon, you will be neglecting higher-order terms, okay.

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So what we want to do is we want to impose small disturbances and what is basically allows me to do is this order epsilon disturbance allows the linearization of the governing equations. So the original equations will typically be nonlinear, okay and since you are talking only about small disturbances, what you will be doing is linearization, that is something which you also saw. You have begun with a nonlinear system.

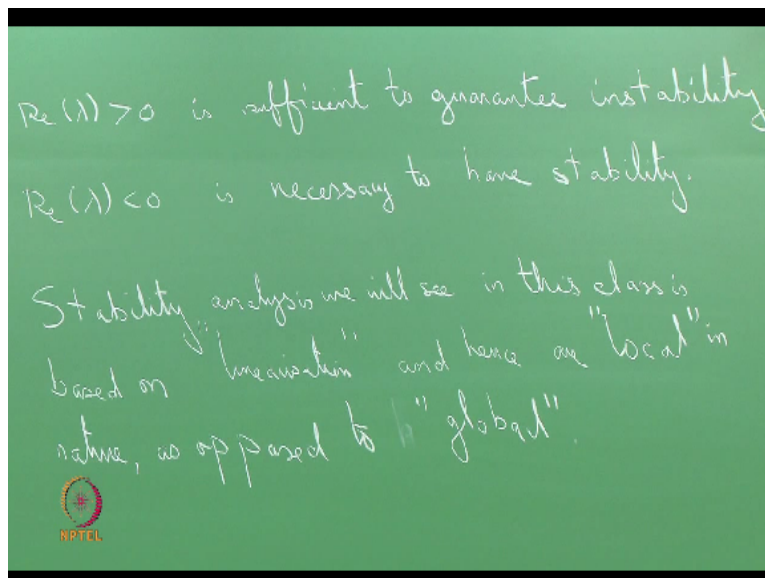
And you linearized it because you are giving only small disturbances, rather what you do is, you do a Taylor series expansion and you need only the first order term. You do not go beyond the first-order term. You do not take higher-order terms. Rather higher-order terms will be nonlinear and then we look at the growth rate of the disturbances. Now growth rate, the disturbances, growth rate, growth or decay rate is given is exponential in time.

Derivative of the form $e^{\lambda t}$ and if λ and since λ will be some eigenvalue of some linear operator which you will see. λ will turn out to be something like an eigenvalue. If the real part of λ is negative, then it is going to decay and you have a stable system. If the real part of λ is positive, it is going to grow, okay. So basically what this means is, the λ s will be say the eigenvalues of a linear operator if the real part of λ is negative, the steady-state is stable and if the real part of λ is positive, it is unstable.

There is just one subtle thing which I want to mention here that when you are doing this calculation, if it turns out that the real part of lambda is positive that means even when you give a small disturbance, it is unstable. So when you give any disturbance, the last disturbance, it will be unstable.

So if the real part of lambda is > 0 , you can definitely conclude that the system is unstable, okay for all disturbances but if the real part of lambda is < 0 , you only know where it is stable for small disturbances but somehow you give the big disturbance, it could be unstable, okay. So you have to be careful here. So whatever I am doing here is in the context of small disturbances, okay.

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So real part of lambda being > 0 is sufficient to guarantee instability while real part of lambda is < 0 is necessary to have stability, that is to say you can have, the condition can be a necessary condition or sufficient condition for something to happen. I am just trying to tell you that real part of lambda is > 0 is sufficient. If it is satisfied, your guarantee is unstable, that is enough, you do not have to do anything else in life.

If this is < 0 , you only know that the necessary condition has been satisfied. It is now assuring you that it will be unstable because of this thing of small disturbance. So whatever stability we

are going to be doing is actually going to be based on those linearized analysis. So whatever we are going to be doing in this course is going to be based on those linearized analysis.

What this means is these are what are called local stability conditions, okay. That is only restricted to small disturbances, okay. So the stability analyses we will see in this class is based on linearization and hence are local in nature as opposed to, what are the other one? Global, okay. So whatever stability we are talking about is the local stability condition or linearized stability condition, okay.

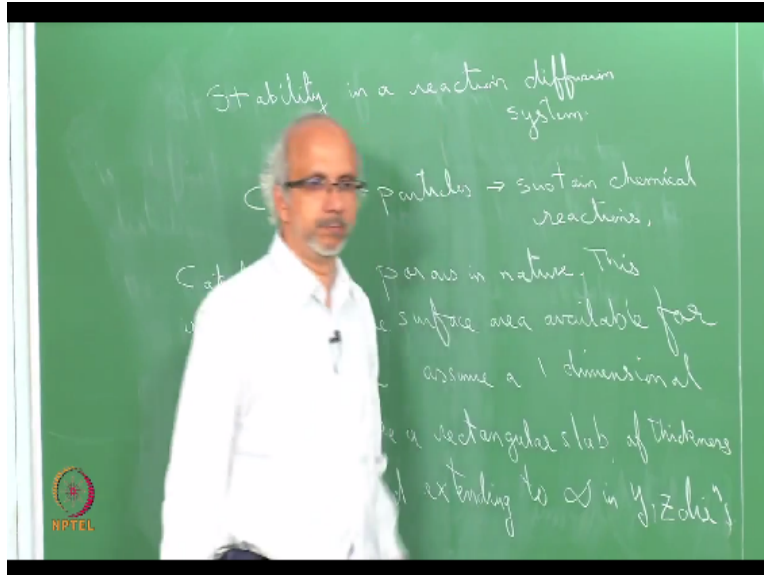
So the analysis is called linearized stability analysis. So it turns out these eigenvalues which are going to basically distract stability, they are going to be dependent upon your operating conditions, your flow rate or your temperature or your this thing concentration and as you vary the parameter, these eigenvalues can actually change from having a negative real part or positive real part.

The growth rate, I want to use the more general term, the growth rate, which basically tells you how disturbances at a particular point change of time, okay, they can change from decay to growth and that is the thing I get interested in. We are trying to find out those critical values when that is going to be a change in the behaviour of the system, okay. So that is basically, this is the mathematical framework.

We spoke something in English, now we are trying to put things in mathematical framework. So given any problem, you can actually work and proceed and address the question of finding the stability, okay because that is the advantage of doing mathematics. You can apply to any system. So it helps you generalize things, okay.

So what we will do today is work on a particular problem which is basically going to take you to a partial differential equation but it is not a flow problem, okay and then we will do a flow problem later on because normally when you do a flow problem in a stability, it is more than 1 equation, so we will just go to slowly adopt the complexity.

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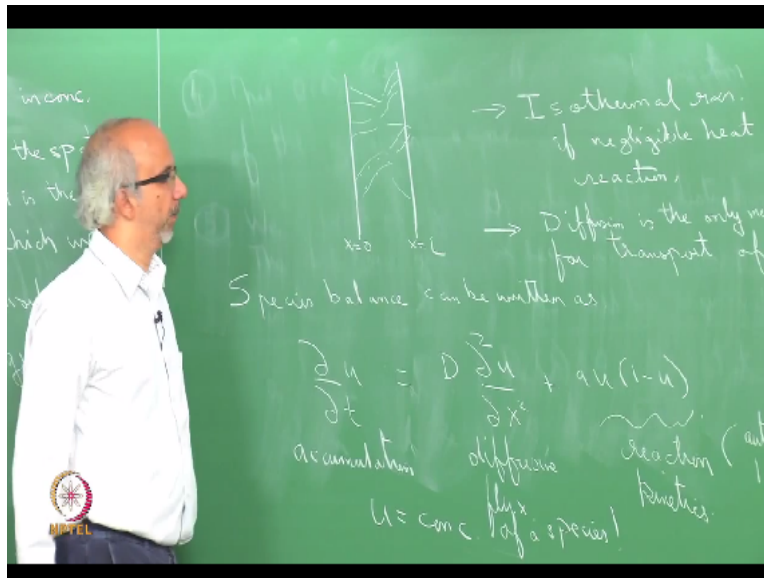
So I am going to talk about stability in a reaction diffusion system, okay. So it belongs to mechanical engineering department to have a chemical engineering example and one of the reasons why I am choosing this example is because I only have to deal with 1 variable either a concentration or temperature. So in this case, it is the concentration. See the catalysts particles which sustain chemical reactions.

And most of you know that catalyst exist, we have done this in our course in chemistry what it does is it basically provides an alternative path for the reaction to take place and makes the reaction go faster, okay. So but the thing is the catalyst is usually deposited on a surface and provides the site for a reaction to take place, okay. Now in order for you to maximise the surface area available for the reaction to occur, what is normally done is there are these catalysts are usually very porous, okay.

So basically what I am saying is the catalyst are porous in nature and this is to maximise the surface area available for reaction, okay. So we will keep life simple and rather than to talk about a spherical particle, we will just say that the particle is a rectangular slab, okay. So imagine, just for the sake of working with Cartesian in geometry, you can work with spherical coordinates. We assume 1-dimensional program, because I just want to illustrate some ideas dimensional problem.

You see my 1-dimensional system which means take a rectangular slab of thickness L in the x direction and extending to infinity in the y and z directions, okay. So I am just extending my infinity in other directions. So what this helps me do is keep my life simple, that is I am just going to worry about variations in the x -direction and since I am talking about stability problem, I want to worry about the time dependency as well, okay.

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So now I am just going to draw the slab here. So this is porous, all kinds of pores all over the place. Some random network of pores will be there and this is a porous solid. So the transport of gas assuming this is a gaseous reaction which takes place on a solid surface, transport of gas inside the solid is going to be only by diffusion, okay. There is not going to be any great velocity inside this pore.

So what I am trying to say here is that the only flux which is going to transport this pieces inside the slab is the diffusion process, okay. We are also going to keep life simple and say that there is no exothermicity and so we are talking about the temperature being constant, okay. So point is isothermal reaction, okay, if we have a negligible heat of reaction and diffusion is the only mechanism for transport of mass, okay.

Now you can write down the governing equations in many different ways but we will just do a shortcut in the sense you know how a species balance looks, okay. You have the convective term,

you have the diffusive term, you have the accumulation term and you have the generation term. So we will just simplify things here. We just say that there is no convection, so only the accumulation term.

The species balance can be written as the partial derivative of $u = \dots$, okay. In some sense, this is way of transport theorem for you. I am doing a species balance here. I am doing it for a small infinitesimal controlled volume. What is this term represent? This term represents the, what is this? The accumulation term, okay. This is flux, okay, because of only diffusion. Convection I am saying is not present.

When we did the Navier-Stokes equation, you have the convective term on the left-hand side. We only had the viscous transport here. So this is your diffusive flux. So basically if you have your overall species balance which you must have done in one of your earlier courses, you will write it down and you drop of terms which do not exist, then you will get this equation, that is the idea.

I am dropping up all the velocity terms that was off. I have diffusion only in the x direction. The y and z direction, I have taken it to be infinity, so I do not worry about it and this here I am just saying is my reaction kinetics. So this kind of reaction kinetics would actually arise when you have an autocatalytic reaction, okay. So this is you have used things like first order reactions, second order.

If it had been the first order reaction, you would had just u or something like that but since it is an upper catalytic reaction in this $u \cdot 1 - u$. So u is basically representing something like a concentration, okay. So here u is concentration of a species. Clearly this is going to be subject to some boundary conditions and the boundary conditions are taken as $u=0$ at $x=0$ and L .

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$u^{ss} \rightarrow \text{implies } \frac{du^{ss}}{dt} = 0$
 $0 = D \frac{d^2 u^{ss}}{dx^2} + u^{ss}(1-u^{ss}), \text{ subject to } u^{ss} = 0, \text{ at } x=0, L$
 if we look for a spatially homogeneous solution, $\frac{d^2 u^{ss}}{dx^2} = 0 \Rightarrow u^{ss}(1-u^{ss}) = 0$ or $u^{ss} = 0$ or 1
 $u^{ss} = 0$ is the only spatially homogeneous solⁿ.

So the thickness of the slab is L , okay. The thickness of the slab is L and both the ends, I will just say u is 0. So that is my governing equation. So what I did is I just did my first step which is write out the governing equation for the system. So I have a catalytic reaction which is isothermal taking place in a slab. I do not have any temperature, so isothermal, no energy balance.

I only need to worry about how the concentration is changing, okay and I need to forget about velocity because there is no convection inside the porous catalyst, okay. It is very negligible. So now the next thing is we need to find the steady-state, right. So for the steady-state, what do you do? Steady-state means you need to put u^{ss} implies d/dt of u^{ss} is 0 which means..., okay subject to...

So since I am looking at a steady-state, the time derivative goes off and my steady-state has to satisfy that equation. So one of the reasons why we actually chose this problem, so one steady-state which immediately pops out is one can be spatially uniform. Supposing you do not have any variation in x direction. Suppose you do not have any variation in the x direction, then this second derivative is going to be 0.

So it is the spatially uniform state or homogenous state where the concentration everywhere inside my pallet is equal. So what kind of a spatially homogenous solution can this system have?

Clearly if this is 0, then u_{ss} could be 0 or it could be 1, okay. So if we look for a spatially homogenous solution, okay, then $d^2 u_{ss}/dx^2 = 0$ will imply $u_{ss} \cdot 1 - u_{ss} = 0$ or $u_{ss} = 0$ or 1 but then your solution should also satisfy the boundary conditions, okay.

So this guy $u_{ss} = 0$ satisfies the boundary conditions whereas $u_{ss} = 1$ does not satisfy the boundary conditions. So $u_{ss} = 1$ is not a solution. The only thing that is possible is $u_{ss} = 0$ is the only solution possible. You understand? So $u_{ss} = 0$ is the only spatially homogenous solution, okay. So my question now is when would the concentration inside my catalyst be spatially uniform, okay? I mean this is a possible solution.

So now what are the different processes which are actually taking place inside your system. One is you have the diffusive process and one is you have the reaction process, okay. So if the diffusion is very very fast, diffusion remember works to make things spatially uniform. So basically the diffusion is very very fast. Your concentration is going to become uniform. Whereas if the diffusion is slow, you are going to have, you can see the concentration gradient.

But this is just English, diffusion being fast and diffusion being small. What you want to do is so in relation to the rate of reaction, I expect that if the diffusion is larger than a critical value, I expect that $u = 0$ is going to be, $u_{ss} = 0$ is going to be something which you can observe because even if there was some disturbance, diffusion is going to make it even. Whereas if there is a disturbance and if diffusion is very slow, there will be a non-uniform solution, okay.

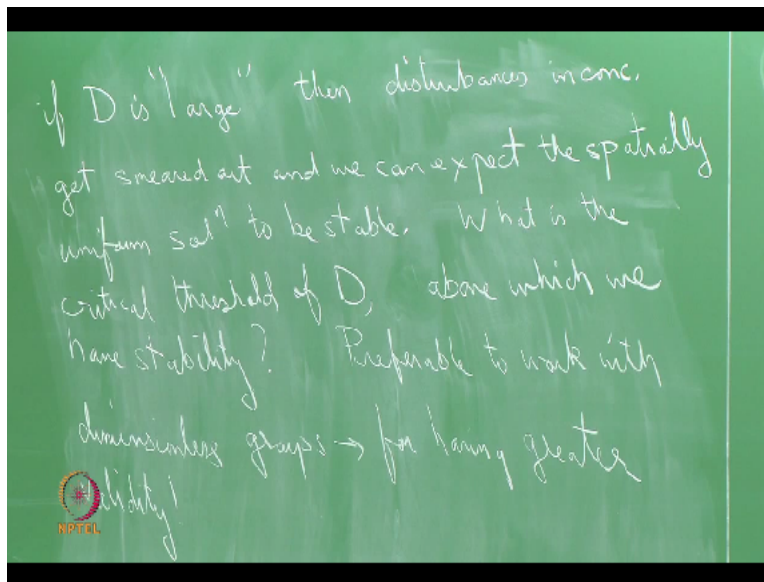
So there will be a variation of concentration inside the catalyst pallet. So that is the question which you are trying to answer. We are trying to find out whether there is some kind of, what is the critical value quantitatively, can I quantify this? Thus where you are able to quantify in terms of the Reynold's number, 2100, okay, can I quantify the value of those diffusion coefficient in some kind of a dimensionless group which will tell me when is this stable, when is this unstable.

So that is the question, okay and the reason why I talked about diffusion is because at the end of the day, what all mathematics tells us has to be in line with whatever our physics tells us. It is not that they are 2 completely different things. As engineers, we have to put mathematics and physics

together, okay. So what I have give you is a possible solution which is spatially homogenous which $u_{ss}=0$, it satisfies the differential equation, satisfies the boundary condition, okay.

And I am telling you that look this is a spatially homogenous solution. I expect the solution to be stable when diffusion is very fast as compared to reaction, okay. But it is not a critical threshold value which decides what is fast and what is slow and that is what mathematics will tell us, okay and that is what we are going to find out by doing the linear stability analysis. So now what we are going to do is, we are going to assume, okay. So let me write this down.

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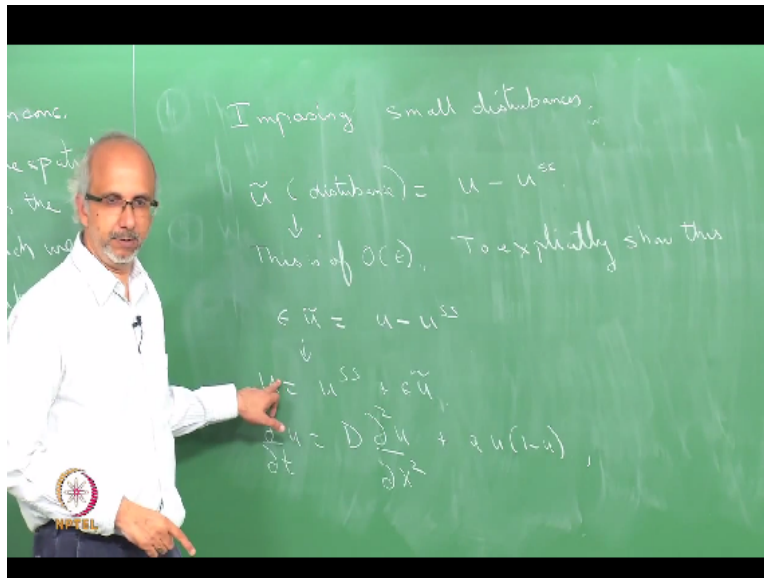


If D is large, I am going to put this in the inverted commas because I want to compare that with something else which has the same units (D) (30:23) okay. D is large, then disturbances in the concentration gets smeared out and we can expect spatially uniform solution to be stable, okay. When D is large, means what? D is larger. So what is the critical threshold of D above which we have stability, that is the question, okay.

And of course one should not talk in terms of D because the diffusion coefficient will depend upon your slab and all that. It is good to work in dimensional coordinates, okay. It is preferable to work with dimensionless groups for having greater validity, that is what I want. Otherwise you will say diffusion specific to a particular system rather than in a dimensionless group, then it becomes more general, okay.

So let us go the next step. So this is the first step, write out the governing equation, I did not derive it (()) (32:47) I think we just wrote out the steady-state. Now we have to do the linearization, right. So I just want to mention, this corresponds to $x=0$ here and $x=L$ here where L was my thickness on the slab.

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So what we are going to do is look at imposing small disturbances and what were these disturbances measure? They measure the deviation from the steady-state, okay. The disturbance basically tells you how far the system is away from the steady-state. Your steady-state is $u^{ss}=0$. So now I am going to, this is my disturbance variable, I am just putting the \sim on top to signify it is a disturbance and this tells me how far is u from the steady-state, okay.

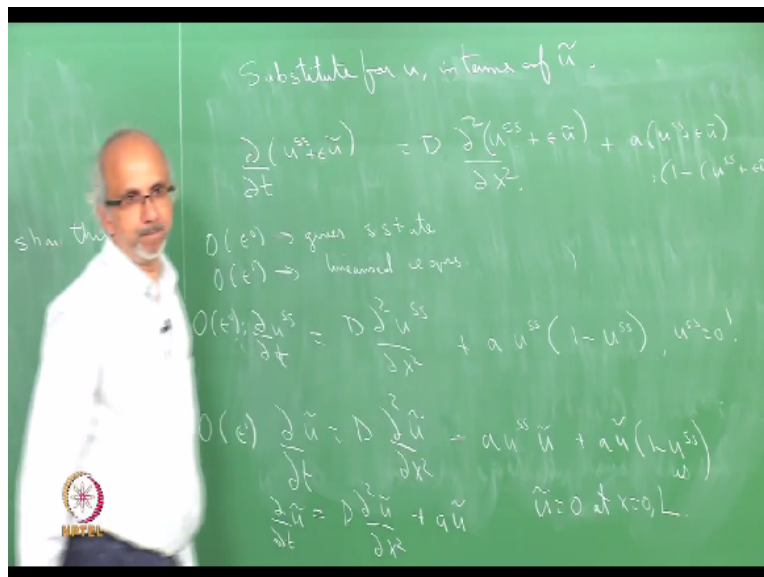
U is the actual concentration and u^{ss} is the steady-state concentration. In this case of course u^{ss} is allowed to be 0, well you could have a problem where u^{ss} is not 0, okay. So I mean just to keep things general, I am writing it like this. So I have $u\sim$ written as $u - u^{ss}$ and what I am going to ask you remember is if this is of order epsilon, this is very small, okay. So if it is order epsilon, I may want to specify that it is of order epsilon by writing it as, to explicitly show this I can write this as $\epsilon u\sim = u - u^{ss}$ where now $u\sim$ will be of order 1 because $\epsilon u\sim$ is of order epsilon, okay.

So this is to explicitly show that this is of order epsilon. I just want to put things in perspective to what you have already done in perturbation analysis. So now it is like saying I am taking u as $u^{ss} + \epsilon u_1$, sorry $u \sim$, okay. This is just to make you relate what you did in your regular perturbation series, you sought u as $u^{ss} + \epsilon u \sim$ etc., okay. In the absence of disturbances, it is u^{ss} .

Now epsilon tells you the mild of the disturbance, there epsilon told you something about the parameter value, okay. So we write it like this. Now I just have to substitute this in my differential equation, okay. I need to substitute this particular form in my differential equation and since I am considering only small deviations, I am going to linearize the term.

The only term which was nonlinear is my reaction term which has quadratic dependency u^2/u , okay. So let me just go back and write those equations here equals, this is my equation, it is a squared, maybe I should just write it here itself, okay, wait a second. That is u , and I am going to substitute for u this expression $u^{ss} + \epsilon u \sim$, okay.

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Substitute for u , in terms of $u \sim$, what you get d/dt of $u^{ss} + \epsilon u \sim = d^2/dx^2 (u^{ss} + \epsilon u \sim) + a(u^{ss} + \epsilon u \sim) / (1 - (u^{ss} + \epsilon u \sim)^2)$, okay. This is multiplying that. What I want to do is group all the terms together of order epsilon to the power 0 and of order epsilon. Order epsilon to the power 0 will be my base state, my steady-state solution. Order epsilon to the power 1 will be my

linearized solution because I am going to basically take only the linear terms, okay.

Order epsilon to the power 0 gives a steady-state and should give the steady-state. Order epsilon to the power 1 should give the linearized equations, okay. So let us just do that. So I have d at order epsilon to the power 0, d/dt of $u_{ss} = d^2 u_{ss}/dx^2 + a u_{ss}(1 - u_{ss})$. That is what I get. This multiplied by this will give me epsilon term, this multiplied by this gives me the 0th order term, okay.

This is not x , okay and this is multiplied by this will give me order epsilon. So this is my steady-state solution about which I am doing the linearization, okay. Because the steady-state goes out to 0 and the solution we are looking at is $u_{ss} = 0$ which satisfies the boundary conditions. What about the order epsilon to the power 1 term? I get d/dt of $u \sim d^2 u \sim /dx^2 + a u \sim (1 - u_{ss})$, now I have $a u \sim + a u \sim (1 - u_{ss})$, okay.

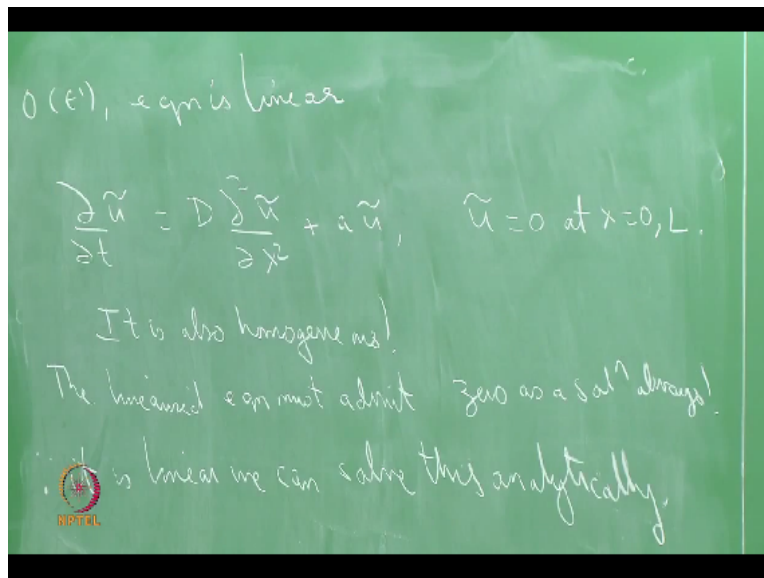
When I have this multiplying this, I have one term and this multiplying this, I have the other term. The other term is of order epsilon squared, so I neglected. Clearly now what I am going to do is use the information which I already have about u_{ss} , that is why you did your perturbation series analysis. You want to use this information about the steady-state being 0 and for steady-state = 0, and then I will find, is that okay?

“Professor - student conversation starts” (()) (40:40) yes, -, what is this? Second term is. This is - here. The second term should be (()) (40:54) $a u \sim (1 - u_{ss})$, it looks okay to me. Second term. This one? Yes, yes. Second term should be negative, you are right. This should be negative, yes, you are right, that is negative. Yes. **“Professor - student conversation ends”**

Now put $u_{ss} = 0$, okay and your linearized equation is d/dt of $u \sim = d^2 u \sim /dx^2 + a u \sim$, that is your equation at order epsilon to the power 1 and what are the boundary conditions? The boundary conditions are going to be u is going to satisfy 0 0. U steady-state satisfies 0 0, so $u \sim$ also have to satisfy 0 0 at the boundary, okay and $u \sim = 0$ at $x = 0, L$, okay. So this comes for the boundary condition, you have to put this perturbation again in the boundary condition, you get this.

What I want to emphasize here is that whenever, that is the linear equation for u because that is what we have done. We essentially done a linearization. You could have done those linearization using Jacobian which is what was discussed last time. You will get the same result, okay. You should do that and verify for yourself.

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So at order epsilon to the power 1, the equation is linear and what do I get? A $u \sim$ and $u \sim = 0$ at $x=0, L$ and not only is a linear, it is also homogenous and I think if you do a linearization, whenever you are working out a problem, after doing the linearization and after looking at things at order epsilon to the power 1, if you find that your equation is not linear, then something is wrong, what you got is wrong.

You will find that there is a non-homogeneity, that means something is wrong. The point I am trying to make here is that the linearized equation should always admit 0 as a solution, okay. So the linearized equation must admit 0 as a solution always, so that is a simple check you can make. Just because it admits 0 as a solution, does not mean you have it right but if it does not admit, it is wrong, okay.

So I think that is the only thing you can do. So what I am trying to tell you is that this is linear and homogenous and now once I started off with the nonlinear problem, I got a steady-state, I

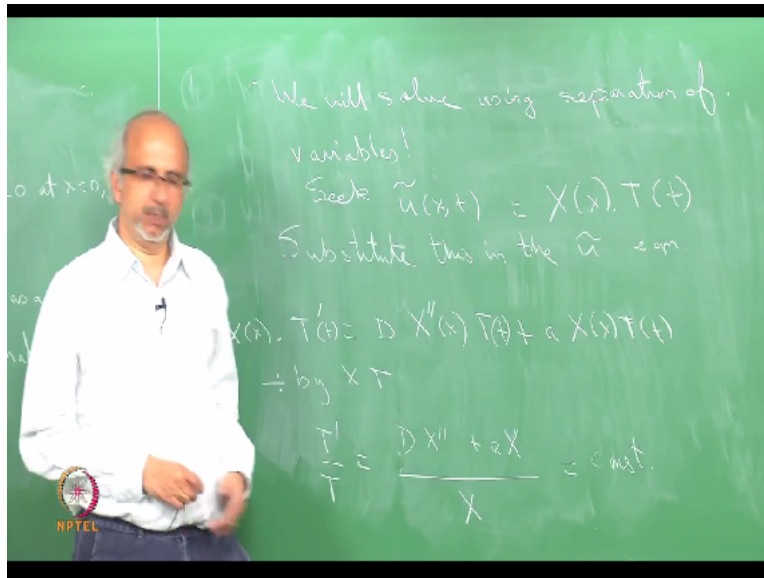
have done a linearization and now as a linear equation, I am kind of comfortable, I am in my comfort zone because I know how to solve this equation using some of the things that you people have learnt in your class like separation of variables, okay.

So now I have a linear equation subject to homogenous, my boundary conditions also have to be homogenous. Everything has to be homogenous, only then I can have this. This is something like an eigenvalue problem. If you remember $ax = \lambda x$. $x=0$ is always a solution. The sum values of λ for which we have non-zero solution plus the kind of things we are looking at here, so 0 as a solution must always satisfy this for no matter what the parameters are and what we are trying to find out is, because it is linear, since it is linear, we can solve this analytically.

So for example above is a linear equation, it is a partial differential equation. So this is one level of complexity more than what you did yesterday. Yesterday you did not have those x and y term. You only have the time derivative term after linearization. We get 2 equations. Today, I have only 1 equation, is partial differential. When we start doing fluid flow problems, it is going to be partial differential and more than 1 variable, okay.

And by the way this is also a very relevant of multiphase flow because I am talking about a gas in a solid. So there are 2 phases, right. This is solid and there is a gas. So do not ask me how is this relevant to fluid flow. It is definitely, there is a fluid flowing and there is a solid particle, okay. Now this is a very relevant to fluid flow. I was beginning to justify with myself that this is relevant for this course, I need this, okay. So now how do you go about solving this? Who remembers this calculus course on partial differential equations?

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We will solve right now using separation of variables. So this u is a function of x and t and what I am going to do is, I am going to write seek u is a function of x and t as X of x * T of t , okay, provided the 2 functions, one which depends only on x and the other which depends only on time. What we will do is, what we normally do is, you substitute this in that partial differential equation and get the x dependency, get the time dependency.

And then you will be in the position to understand by looking at the growth rate, the exponential term which I spoke about earlier, whether the thing is stable or unstable, right. So that is what we will do. Substitute this in the, actually this will be u , u equation and what do you get? X of x * T dash= D * X double dash of x * T + a * X of x * T of t , okay. What we do now is, we divide throughout by X , multiply it by T , okay.

Divide by XT and what do you get? T dash/ T = D * X double prime+ aX / X , okay. It is just divided by XT and that is how I get and so the classical argument that this left-hand side is a function only of time, the right-hand side is a function only of X , so the only way these guys can be equal is that this is equal to a constant.

And what this basically tells me is I can solve for this ordinary differential equation which is first order in time. I can solve for this ordinary differential equation for the second order in space and then hope to proceed to getting my solution. So we will do this tomorrow and we will wrap up

this problem, okay.